Phase diagram of a Bose-Fermi mixture in a one-dimensional optical lattice in terms of fidelity and entanglement

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We study the ground-state phase diagram of a Bose-Fermi mixture loaded in a one-dimensional optical lattice by computing the ground-state fidelity and quantum entanglement. We find that the fidelity is able to signal quantum phase transitions between the Luttinger liquid phase, the density-wave phase, and the phase separation state of the system; and the concurrence can be used to signal the transition between the density-wave phase and the Ising phase.

Ultra-cold atomic gas loaded in optical lattice are attracting more and more attentions due to ambitions of getting deep insight into some essential physical phenomenons, such as quantum phase transitions (QPTs),[1] in the condensed matter physics. The prediction[2] and the successful observation[3] of the QPT from a superfluid to a Mott-insulator was one of the greatest works in this field. Quite recently, experimental progresses are very promising for studying more non-trivial quantum phases in clod atomic systems. For example, bosonic and fermionic atoms can simultaneously be trapped in optical lattice in a controllable way. This ultra-cold atomic system, the so-called Bose-Fermi mixture, often reminds people of the solid state systems including the electron-phonon interaction. The latter have been studied for a long period and have a complicated quantum phase diagram. So to explore new possible phases in this system becomes an interesting theoretical problem. Along this line, several works had been done.[4,5,6,7,8] It is worthwhile to mention that Lode Pollet *et. al.* recently studied the ground-state phase diagram of a Bose-Fermi mixture loaded in a one-dimensional (1D) optical lattice by using quantum Monte Carlo (QMC) simulations.[8] Several phases, including Luttinger liquid (LL) phase, density wave (DW) phase, phase separation (PS) state, and Ising phase, are predicted.

In recent years, some concepts emerging in the quantum information theory[9] are extensively used to study the critical phenomena in quantum many-body systems. One of the typical examples is the entanglement. Many efforts have been made to the relation between the entanglement and QPTs.[10,11,12] Quite recently, the fidelity, as a measure of similarity between states, was proposed to study the critical phenomena. The motivation is very simple: a dramatic change in the structure of the ground state around the quantum critical point should result in a great difference between the two ground states on the both sides of the critical point. The fidelity has been successfully applied to study the spin, fermionic, and most recently bosonic systems.[13,14,15,16,17,18,19,20,21] Compared with entanglement, the fidelity is purely a geometrical quantity; an obvious advantage is that in analyzing the QPTs it does not require a priori knowledge of the order parameter and the symmetry of the system.

In this paper we try to study the ground-state fidelity and the entanglement of the Bose-Fermi mixture in a 1D optical lattice. The aim is two-folded: one is to test the role of fidelity and entanglement in a more realistic system, the other is to study the ground-state properties of the Bose-Fermi mixture. Follow Lode Pollet *et. al.*[8], we assume that a mixture of bosonic and fermionic atoms is loaded into a 1D optical lattice, and the temperature is low enough such that quantum degeneracy is achieved. The system is then described by a lowest-band Bose-Fermi Hubbard model,

$$H = -\sum_{i=1}^{N}(t_F c_i^\dagger c_{i+1} + t_B b_i^\dagger b_{i+1} + \text{H.c.})$$

$$+ U_{BF}\sum_{i=1}^{N} c_i^\dagger c_i b_i^\dagger b_i + U_{BB}\sum_{i=1}^{N} b_i^\dagger b_i(b_i^\dagger b_i - 1), \quad (1)$$

where b_i (b_i^+) and c_i (c_i^+) are the bosonic and fermionic annihilation (creation) operators at site i, respectively. Bosons (fermions) can hop from site i to the nearest neighbor site $i \pm 1$ with tunneling amplitude t_B (t_F). Furthermore, a large occupation of bosons on a single site is suppressed by the on-site repulsion interaction U_{BB}. Bosons and fermions can mutually repel or attract each other on each site depending on the sign of U_{BF}. In this paper, we choose $U_{BF} > 0$, and consider the case where both of the bosons and the fermions have a density as: $N_F = N_B = N/2$.

We now briefly introduce the ground-state phase diagram of the model. When the U_{BF} is small enough, the fermions behave as a LL, the interaction between them is induced by the bosons. At the same time, the bosons form an interacting liquid too. So we have a LL of fermions, which weakly interacts a boson liquid. When U_{BB} is small and U_{BF} is large, the system is in the first order unstable to the PS with hard domain walls; in other words the system is separated into two regions: a bosonic region and a fermionic region. When both U_{BB} and U_{BF} are very large, the bosons behave as fermions, which means that the occupation of more than one boson at a single site is not allowed. The model can then be mapped into the 1D XXZ model: $H_{XXZ} = \sum_i J(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J^z \sigma_i^z \sigma_{i+1}^z$, where $J = -(t_B t_F)/U_{BF}$ and $J^z = (t_F^2 + t_B^2)/(2U_{BF}) - t_B^2/(2U_{BB})$[22]. This implies that there are three phases in this limit: the ferromagnetic phase, a gapless DW phase and a gapped Ising phase. In the ferromagnetic phase, boson-boson bonds and
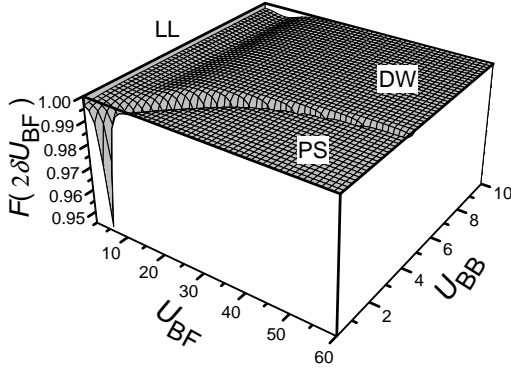
FIG. 1: The obtained fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ when $t_F = 4.0, t_B = 1.0, \delta U_{BF} = 0.5$. It can be observed obviously that there are two phase transition boundary lines indicated by the drop in the fidelity. The phases such as LL, DW, and PS are identified by the comparing this phase diagram with the one which was proposed earlier by the calculation of the correlation functions (see text). $N = 8$ (APBC).

fermion-fermion bonds are favored compared with bonson-fermion bonds due to the larger exchange interactions, this mechanism makes the system form two regions with hard domain walls. So the ferromagnetic phase corresponds to the PS in the mixture. This mechanism is similar to the one appearing in the 1D asymmetric Hubbard model[23,24] where the PS is also occurred when the system is away from half-filling. While in the DW phase and Ising phase, the system always favors bonson-fermion bonds. We could like to emphasis that the PS in the large U_{BB} limit and the one in the small U_{BB} limit are different since that the latter allows the occupation of more than one boson on a single site. In the whole PS region, with the increasing of U_{BB}, the boson repulsion exerts a pressure such that the region occupied by the bosons will grow and at the same time the local density of bosons will decrease.

As mentioned, the fidelity is nothing but the modulus of the overlap of two ground states relative to two different choices of the Hamiltonian parameters. In this paper, we mainly focus on these two:

$$F(2\delta U_{BF}, U_{BF}, U_{BB}) = |\langle\psi_{U_{BF}-\delta U_{BF}}|\psi_{U_{BF}+\delta U_{BF}}\rangle|, \quad (2)$$
$$F(2\delta U_{BB}, U_{BF}, U_{BB}) = |\langle\psi_{U_{BB}-\delta U_{BB}}|\psi_{U_{BB}+\delta U_{BB}}\rangle|, \quad (3)$$

in which $|\psi_\lambda\rangle$ stands for the ground state of the Hamiltonian (1) with the parameter λ, and is calculated by the Lanczos method for a finite sample. To avoid the ground-state level crossing, anti-periodic boundary conditions (APBCs) are applied for system size $N = 4n$ and periodic boundary conditions (PBCs) for $N = 4n + 2$, where n is an integer. According to the original motivation of the fidelity, a drop in the fidelity of two ground states separated by two lightly different parameters is expected to be a signature of the QPT.

In Fig. 1, we show one of our main results, i.e. the fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ defined on the $U_{BB} - U_{BF}$ plane. Compare this figure with Fig. 4 of Ref. 8, perfect similarity can be observed. The boundary lines of phase transitions between the LL, the DW and the PS are clearly indicated by the drop of

the fidelity. We would like to emphasis that the phase diagram presented here is obtained in such a small cluster and without any knowledge of the correlation properties of the system. It is also clearly observed that the drop of the fidelity along the phase transition line between the DW and PS phases becomes deeper and deeper as the interaction decreases. This phenomenon indicates that although the phase transition is within the same class but the similarity of the ground state is changing along this line.

However, the phase transition, as reported in Ref. 8, between the DW and the Ising phases is not indicated in Fig. 1. According to the effective model, i.e. 1D XXZ model, this transition belongs to the KT universality class.[8,25] Lode Pollet et. al.[8] did numerical calculation of the correlation functions in a relatively larger system ($N \sim 30$) by the QMC simulations and claimed that a true long-range order may exist in the Ising phase. It is highly difficult for us to make a scaling analysis of the correlation functions by the Lanczos method. However, the 1D XXZ[26] model provides us a clue to investigate this problem. It was reported that the concurrence,[27] as a measure of entanglement between two qubits, reaches maximum at the SU(2) point[11] of the XXZ model. This maximum point corresponds to the transition point between the DW and the Ising phases.

The concurrence in the spin models can be calculated in the following way. Due to the global SU(2) symmetry of the XXZ model, the z-component of the total spin of the system is a good quantum number, the reduced density matrix $\rho_{i,i+1}$ of two neighboring spins has the form

$$\rho_{i,i+1} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w & z^* & 0 \\ 0 & z & w & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}, \quad (4)$$

in the spin basis $|\uparrow\uparrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle$. The elements in the reduced density matrix $\rho_{i,i+1}$ can be obtained from the correlation functions

$$u^\pm = \frac{1}{4}(1 \pm 2\langle\sigma_i^z\rangle + \langle\sigma_i^z\sigma_{i+1}^z\rangle), \quad (5)$$

$$w = \frac{1}{4}(1 - \langle\sigma_i^z\sigma_{i+1}^z\rangle), \quad (6)$$

$$z = \frac{1}{4}(\langle\sigma_i^x\sigma_{i+1}^x\rangle + \langle\sigma_i^y\sigma_{i+1}^y\rangle + i\langle\sigma_i^x\sigma_{i+1}^y\rangle - i\langle\sigma_i^y\sigma_{i+1}^x\rangle). \quad (7)$$

All the information needed is contained in the reduced density matrix, from which the concurrence is readily obtained as[?]

$$C = 2\max\left[0, |z| - \sqrt{u^+u^-}\right], \quad (8)$$

which can be expressed in terms of the correlation functions and the magnetization by using equation (5), (6) and (7).

The concurrence is only valid for two-qubit system. For the Bose-Fermi Hubbard model, the double occupation of two particles is almost not allowed, the state of the two neighboring sites can be described by four basis $|ff\rangle, |bf\rangle, |fb\rangle, |bb\rangle$ where f (b) represents there is only one fermion (boson) on a single site. So we can associate a pseudo-spin "up" ("down") with the "f" ("b"). Then the equations described above can
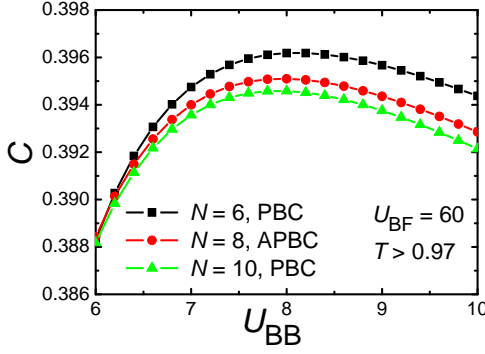
FIG. 2: The obtained concurrence in the DW phase where $t_F = 4.0, t_B = 1.0$. The concurrence of the $N = 6$ ($N = 8$) had been reduced by 0.029 (0.009) in order to make the results reside in the same region in figure. All other parameters are indicated in the figure.

also be perfectly applied to the Bose-Fermi Hubbard model. In other words, if we calculate the trace of the reduced matrix of two nearest sites, which reads $T = \mathrm{Tr}\rho_{i,i+1}$, then T must equal to 1 in this limit. While T only approximately equals 1, when U_{BB} and U_{BF} are not infinite but large. As long as $(1 - T)$ is small enough the concurrence calculated by Eq. (8) is a good characterization of entanglement between two sites. In this way, we are able to calculate the concurrence in the Bose-Fermi mixtures approximately. This kind of treatment was also used by some other group recently[28]. Obviously, as expected a maximum is clearly observed in the behavior of the concurrent, which indicates a QPT point. It is important to point out that the variety of the concurrence is not a dramatic one in the whole DW region. Using the exact solution of the XXZ chain, the phase transition from the DW phase to the Ising phase should occur at $-J = J^z$, i. e. $U_{BB} = 6.7$ for $t_F = 4.0, t_B = 1.0, U_{BF} = 60$. But according to the obtained concurrence, the max point U_{BB}^{max} approximately equals to 7.7. The discrepancy comes from the approximations made and the size effect.

Some skeptical readers may wonder why other kinds of measurements of the entanglement, for example the von Neumann entropy, are not calculated here since these kinds of measurements are more suitable for the Bose-Fermi Hubbard model at the first glance of their definitions. We actually calculated von Neumann entrpy though we did not show here. But it turns out that these quantities are more difficult to witness the phase transition between the DW and Ising phase.

After all the analysis, we contribute the missing of the phase transition signature between the DW phase and the Ising phase in the fidelity to two reasons. The first one is that this kind of transition is actually a very weak one, which means that the change of the ground state around the critical point is not dramatic, at least in the finite size system according to our results. The second one is that, as reported before, the fidelity may not be a good indicator of those transitions of infinite order, such as KT transitions.[17] However, further studies are definitely needed in order to answer the question completely!

We also calculated the fidelity $F(2\delta U_{BB}, U_{BF}, U_{BB})$ which
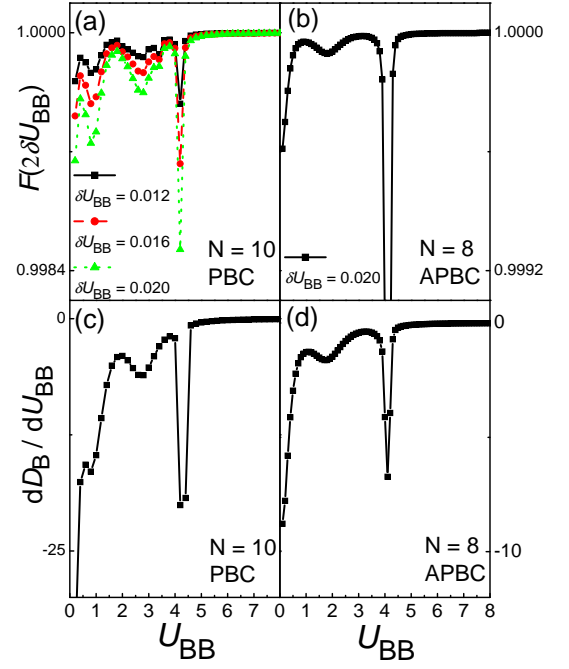

FIG. 3: The obtained fidelity $F(2\delta U_{BB}, U_{BF}, U_{BB})$ (a), (b) and the first order derivative of the local density of boson (see text)(c), (d) when $t_F = 4.0, t_B = 1.0, U_{BF} = 60.0$. All other parameters are indicated in the figure.

can signal the transition between the PS phase and DW phase too. As you can see in the Fig. 3, the most dramatic drop in the fidelity is in correspondence with the phase transition point between the PS state and the DW phase. The critical point find here is consistence with the one found in the Fig. 1. In addition, some other drops in the fidelity can be observed in the PS region. These drops are related to the changing rate of the local density of boson. To show this, we define the local density of boson as,

$$D_B = \langle \frac{1}{N} \sum_{i=1}^{N} b_i^\dagger b_i (b_i^\dagger b_i - 1) \rangle, \qquad (9)$$

and its first order derivative is calculated. Comparing Fig. 3 (a) and Fig. 3 (b) with Fig. 3 (c) and Fig. 3 (d) respectively, every drop in the fidelity has its company, a drop in the derivative of the local density of boson. This relation can be understood by the dramatic change of the local density of boson will lead to a big change of the ground state wave-function, and then will make the fidelity decrease greatly. The drop of the fidelity at the QPT point between the PS state and DW phase can also be thought like this way. These observations strongly imply that the transition between PS phase and DW phase is within the Landau's symmetry breaking theory and a first order one. Furthermore, it is easy to notice that the phase transition point is not affected by the system size and the boundary conditions used, but the drops found in the PS phase is strongly affected, which indicates that these drops may be a size effect and can not be identified as phase transitions. Furthermore, the transition between DW phase and

Ising phase is not observed again!

In summary, we calculated the fidelity $F(2\delta U_{BF}, U_{BF}, U_{BB})$ and $F(2\delta U_{BB}, U_{BF}, U_{BB})$ of the 1D Bose-Fermi Hubbard model, which can be used to describe low-temperature physics of the atomic Bose-Fermi mixtures loaded in 1D optical lattices. It is showed that although the ground state phase diagram of this system is complicated, and the fidelity may be a good tool to study the phase transitions without a priori knowledge of the order parameter and the symmetry of the system. But one should be very careful because the fidelity may fail for the transition which is belong to the KT-like type, for example, the transition between DW phase and Ising phase in this system. We also calculate the concurrence in the DW phase.

The result indicate a QPT may exist in the DW phase although the fidelity have no singulary at this transition point.

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